1,10-Phenanthroline
66-71-7 | DTXSID1025857

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 127 °C

Global applicability domain: Inside

Local applicability domain index: 5.83e-01

Confidence level: 5.40e-01

Nearest Neighbors from the Training Set

Image not found
Benzo[c]cinnoline
Measured: 158
Predicted: 141

Image not found
Fenazaquin
Measured: 78.5
Predicted: 98.7

Image not found
Proquazone
Measured: 138
Predicted: 122

Image not found
Clotrimazole
Measured: 148
Predicted: 132

Image not found
Trimeprazine
Measured: 68.0
Predicted: 104